

L Number	Hits	Search Text	DB	Time stamp
1	110	acorus near2 calamus	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:35
3	21	(acorus near2 calamus) and \$4asarone	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:32
4	89	(acorus near2 calamus) not \$4asarone	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:36
5	149	sweet near2 flag	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:36
6	406282	hydrogenat\$6 or h2!	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:37
7	13	((acorus near2 calamus) or (sweet near2 flag)) same (hydrogenat\$6 or h2!)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:37
2	38	\$4asarone	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:38

09/652,376

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| | | |
|--------------|----|---|
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| NEWS | 2 | "Ask CAS" for self-help around the clock |
| NEWS | 3 | May 12 EXTEND option available in structure searching |
| NEWS | 4 | May 12 Polymer links for the POLYLINK command completed in REGISTRY |
| NEWS | 5 | May 27 New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus |
| NEWS | 6 | May 27 CAplus super roles and document types searchable in REGISTRY |
| NEWS | 7 | Jun 28 Additional enzyme-catalyzed reactions added to CASREACT |
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| NEWS | 10 | Jul 30 BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting |
| NEWS | 11 | AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields |
| NEWS | 12 | AUG 02 CAplus and CA patent records enhanced with European and Japan Patent Office Classifications |
| NEWS | 13 | AUG 02 STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting |
| NEWS | 14 | AUG 02 The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available |
| NEWS | 15 | AUG 04 Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004 |
| NEWS EXPRESS | | JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004 |
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FILE 'HOME' ENTERED AT 17:48:27 ON 19 AUG 2004

09/652,376

=> file reg
COST IN U.S. DOLLARS
SINCE FILE ENTRY TOTAL
SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 17:48:38 ON 19 AUG 2004
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 18 AUG 2004 HIGHEST RN 728239-10-9
DICTIONARY FILE UPDATES: 18 AUG 2004 HIGHEST RN 728239-10-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

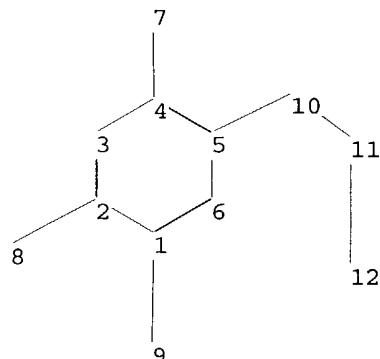
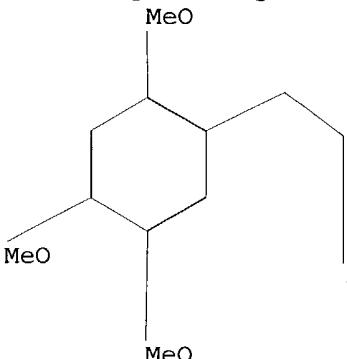
=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END) :end

=> screen 1992 OR 2016 OR 2021 OR 2026 OR 1839

L1 SCREEN CREATED

=>
Uploading C:\Program Files\Stnexp\Queries\09652376.str



chain nodes :
7 8 9 10 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
1-9 2-8 4-7 5-10 10-11 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6

09/652,376

exact bonds :
1-9 2-8 4-7 5-10 10-11 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS

L2 STRUCTURE UPLOADED

=> que L2 NOT L1

L3 QUE L2 NOT L1

=> s 13
SAMPLE SEARCH INITIATED 17:48:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 58 TO ITERATE

100.0% PROCESSED 58 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 704 TO 1616
PROJECTED ANSWERS: 8 TO 329

L4 8 SEA SSS SAM L2 NOT L1

=> s 13 ful
FULL SEARCH INITIATED 17:49:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1215 TO ITERATE

100.0% PROCESSED 1215 ITERATIONS 175 ANSWERS
SEARCH TIME: 00.00.01

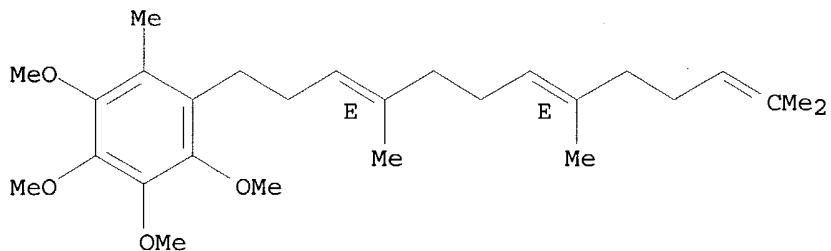
L5 175 SEA SSS FUL L2 NOT L1

=> d scan

L5 175 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzene, 1,2,3,4-tetramethoxy-5-methyl-6-[(3E,7E)-4,8,12-trimethyl-3,7,11-tridecatrienyl]- (9CI)
MF C27 H42 O4

Double bond geometry as shown.

09/652,376



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

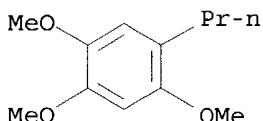
=> s 13 ful css
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FULL SCREEN SEARCH COMPLETED - 1215 TO ITERATE

100.0% PROCESSED 1215 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L6 1 SEA CSS FUL L2 NOT L1

=> d

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 6906-65-6 REGISTRY
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1,2,4-Trimethoxy-5-propylbenzene
CN 1-(2,4,5-Trimethoxyphenyl)propane
CN Dihydroasarone
FS 3D CONCORD
MF C12 H18 O3
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPAT2,
USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP
(Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence);
PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); NORL
(No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13 REFERENCES IN FILE CA (1907 TO DATE)
13 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

09/652,376

=> file caplus caold
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 312.61 | 312.82 |

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=> s 6906-65-6
L7 14 6906-65-6

=> dup rem l7
DUPLICATE IS NOT AVAILABLE IN 'CAOLD'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
PROCESSING COMPLETED FOR L7
L8 14 DUP REM L7 (0 DUPLICATES REMOVED)

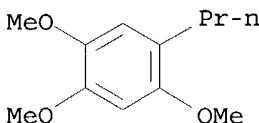
=> d 1-14 bib ab fhitstr

L8 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:777737 CAPLUS
DN 139:292100
TI Formation of neolignan by DDQ mediated dimerization of dihydroasarone
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi
PA Council of Scientific and Industrial Research, India
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2003080551 A1 20031002 WO 2002-IN73 20020327
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI WO 2002-IN73 20020327
OS CASREACT 139:292100
AB The present invention relates to a novel neolignan 3-ethyl-2-methyl-3-(2',4',5'''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-propene and a process for the preparation of high purity, high yield neolignan, α -asarone, and 2,4,5-trimethoxyphenylpropionone from β -asarone or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.
IT 6906-65-6P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic

09/652,376

preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of neolignan by DDQ mediated dimerization of dihydroasarone)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

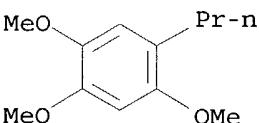


RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:777446 CAPLUS
DN 139:292099
TI DDQ-mediated one step dimerization of β -asarone or β -asarone rich Acorus calamus oil in the formation of novel neolignan
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi
PA Council of Scientific & Industrial Research, India
SO U.S. Pat. Appl. Publ., 20 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------|------|----------|-----------------|----------|
| PI US 2003187306 | A1 | 20031002 | US 2002-108269 | 20020328 |
| US 2004049085 | A1 | 20040311 | US 2003-660556 | 20030912 |
| PRAI US 2002-108269 | B3 | 20020328 | | |

OS CASREACT 139:292099
AB The present invention relates to a novel neolignan, 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-(2',4',5'-trimethoxy)phenyl-1-propene [NEOLASA-I (I)], and a process for the preparation of high purity, higher yield neolignan, α -asarone, 2,4,5-trimethoxy-phenylpropionone from β -asarone (II) or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.
IT 6906-65-6P, Dihydroasarone
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dimerization of, with DDQ; DDQ-mediated one step dimerization of β -asarone or β -asarone rich Acorus calamus oil in the formation of novel neolignans)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

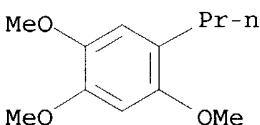


L8 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:524051 CAPLUS
DN 139:90404
TI Process for the preparation of pharmacologically active α -asarone

09/652,376

from toxic β -asarone-rich Acorus calamus oil
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi
PA Council of Scientific & Industrial Research, India
SO U.S., 22 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|-----------------|-----------------|-----------------|----------|
| PI | US 6590127 | B1 | 20030708 | US 2002-107844 | 20020328 |
| | WO 2003082786 | A1 | 20031009 | WO 2002-IN94 | 20020328 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| PRAI | US 2002-107844 | A | 20020328 | | |
| AB | The present invention relates to a process for the preparation of high purity and yield α -asarone, trans-2,4,5-trimethoxycinnamaldehyde, and 2,4,5-trimethoxyphenylpropanone, from β -asarone or β -asarone-rich Acorus calamus oil containing α and γ -asarone by hydrogenation, followed by treatment with a dehydrogenating agent dichlorodicyanobenzoquinone (DDQ) with or without solid support of silica gel or alumina in dry organic solvent. α -Asarone can also be obtained by treating the hydrogenated product of β -asarone or β -asarone-rich A. calamus oil with DDQ in an aqueous organic solvent to obtain an intermediate 2,4,5-trimethoxyphenylpropanone, which in turn is reduced with sodium borohydride to obtain the corresponding 2,4,5-trimethoxyphenylpropanol and followed by final treatment with a dehydrating agent. | | | | |
| IT | 6906-65-6P, Dihydroasarone | | | | |
| | RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pharmacol. active α -asarone by hydrogenation of toxic β -asarone-rich Acorus calamus oil) | | | | |
| RN | 6906-65-6 CAPLUS | | | | |
| CN | Benzene, 1,2,4-trimethoxy-5-propyl- | (7CI, 8CI, 9CI) | (CA INDEX NAME) | | |



RE.CNT 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:717107 CAPLUS
DN 137:234008
TI Production of substituted trans-cinnamaldehydes and yellow dyes from phenylpropane derivatives
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Dogra, Ruchi
PA India
SO U.S. Pat. Appl. Publ., 15 pp.

09/652,376

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|------|--|------------------|----------|
| PI | US 2002133045 | A1 | 20020919 | US 2001-805832 | 20010314 |
| | US 6566557 | B2 | 20030520 | | |
| | GB 2373252 | A1 | 20020918 | GB 2001-6430 | 20010315 |
| | DE 10113506 | A1 | 20020926 | DE 2001-10113506 | 20010320 |
| | BR 2001003269 | A | 20021203 | BR 2001-3269 | 20010322 |
| | FR 2822473 | A1 | 20020927 | FR 2001-3984 | 20010323 |
| | WO 2002072709 | A1 | 20020919 | WO 2001-IN104 | 20010521 |
| | | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | |
| | | RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | |

PRAI US 2001-805832 A 20010314

OS CASREACT 137:234008; MARPAT 137:234008

AB The invention relates to the production of substituted trans-cinnamaldehydes (I, R₁ = trans-CH:CHCHO; R₂, R₃, R₄, R₅, R₆ = H, alkyl, alkoxy, or adjacent groups may form methylenedioxy) by oxidizing the corresponding phenylpropane derivs. using an oxidizing agent such as 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), p-chloranil, pyridinium chlorochromate, tert-BuOOH, or CrO₃ with a catalytic amount of inorg./organic acid (optionally on alumina, celite, and silica gel as a solid support for microwave irradiation); the trans-cinnamaldehydes and natural yellow dyes are obtained in high yield ranging from 68-82%. In an example, yellow 2,4,5-trimethoxycinnamaldehyde was obtained in 84% yield by oxidation of 1-(2,4,5-trimethoxyphenyl)propane in the presence of DDQ and acetic acid.

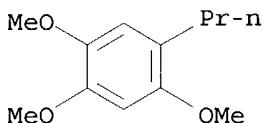
IT 6906-65-6, 1-(2,4,5-Trimethoxyphenyl)propane

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; in production of cinnamaldehydes and yellow dyes by oxidation of phenylpropane derivs.)

RN 6906-65-6 CAPLUS

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:221245 CAPLUS

DN 136:247399

TI Process for the preparation of 1-propyl-2,4,5-trimethoxybenzene from toxic β-asarone of Acorus calamus or from crude calamus oil containing β-asarone

IN Sinha, Arun Kumar

PA Council of Scientific and Industrial Research, India

SO U.S. Pat. Appl. Publ., 16 pp., Division of U.S. Ser. No. 652,376.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|----------------|------|----------|-----------------|----------|
| PI | US 2002035299 | A1 | 20020321 | US 2001-957867 | 20010921 |
| | US 6528041 | B2 | 20030304 | | |
| | CN 1340494 | A | 20020320 | CN 2001-119219 | 20010327 |
| | JP 2002088004 | A2 | 20020327 | JP 2001-101894 | 20010330 |
| | US 2003113275 | A1 | 20030619 | US 2003-338327 | 20030108 |
| PRAI | US 2000-652376 | A3 | 20000831 | | |
| | US 2001-957867 | A3 | 20010921 | | |

OS CASREACT 136:247399

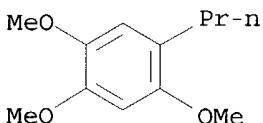
AB The invention relates to a process for the preparation of 1-Propyl-2,4,5-trimethoxybenzene useful as a aroma mol. and as a starting material and intermediate for preparation of various drugs. The process comprises providing crude calamus oil or β -asarone in a solvent; hydrogenating the solution in the presence of a catalyst; filtering the catalyst and removing the solvent under reduced pressure; subjecting the reduced calamus oil to column of silica gel chromatog. using an eluent to obtain the desired product in liquid form with 85-97% purity.

IT 6906-65-6P, Benzene, 1,2,4-trimethoxy-5-propyl-

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-propyl-2,4,5-trimethoxybenzene from toxic β -asarone of Acorus calamus or from crude calamus oil containing β -asarone)

RN 6906-65-6 CAPPLUS

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 6 OF 14 CAPPLUS COPYRIGHT 2004 ACS on STN

AN 2002:710993 CAPPLUS

DN 137:249076

TI Process for preparation of substituted trans-cinnamaldehyde, a natural yellow dye, from phenylpropane derivatives

IN Sinha, Arun Kumar; Joshi, Virendara Prasad; Dogura, Ruci

PA Council of Scientific & Industrial Research, India

SO Jpn. Kokai Tokkyo Koho, 45 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

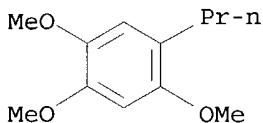
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---------------|------|----------|-----------------|----------|
| PI | JP 2002265407 | A2 | 20020918 | JP 2001-68716 | 20010312 |
| PRAI | JP 2001-68716 | | 20010312 | | |

OS CASREACT 137:249076; MARPAT 137:249076

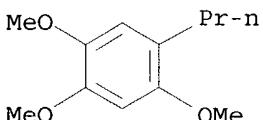
AB A simple and economical process to convert phenylpropane derivs. into corresponding cinnamaldehyde derivs. comprises oxidizing substituted phenylpropane derivs. in presence of a solvent and a catalyst using an oxidizing agent in a mole ratio of 1:1 to 1:8 to the phenylpropane derivs. at a temperature between -15° to 210° for a period of 30 min to 48 h, removing the solvent under reduced pressure and isolating the product to obtain 68-82% of trans-cinnamaldehydes. Thus, a flask containing a mixture of 4-methoxyphenylpropane 2, silica gel 0.5-0.8, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) 7.5 g and 5-8 mL dioxane was placed inside a microwave oven operating at medium power (600 W) and irradiated for 2-8

09/652,376

min to give 68% 4-methoxycinnamaldehyde.
IT 6906-65-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(simple and economical process for preparation of substituted
trans-cinnamaldehyde natural yellow dye from phenylpropane derivs.)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:830461 CAPLUS
DN 136:128585
TI High hypolipidemic activity of saturated side-chain α -asarone
analog
AU Cruz, Adriana; Garduno, Leticia; Salazar, Maria; Martinez, Elizdath; Diaz,
Francisco; Chamorro, German; Tamariz, Joaquin
CS Departamento de Quimica Organica, Escuela Nacional de Ciencias Biologicas,
IPN. Prol. Carpio y Plan de Ayala, Mexico, 11340, Mex.
SO Medicinal Chemistry Research (2001), 10(9), 587-595
CODEN: MCREEB; ISSN: 1054-2523
PB Birkhaeuser Boston
DT Journal
LA English
AB With the aim of evaluating the pharmacophore potential of the side chain
of α -asarone regarding its high hypolipidemic activity,
 α -asarone analogs (I) were evaluated pharmacol. For I, with a
variable-size side chain, significant decreases in serum cholesterol,
LDL-cholesterol, and triglyceride levels and significant increases in
HDL-cholesterol levels were observed in mice. I were even more active than
 α -asarone in reducing cholesterol. The results suggested that the
length and saturated character of the side chain seem to be a key feature in
improving hypolipidemic activity of I.
IT 6906-65-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(high hypolipidemic activity of saturated side-chain α -asarone
analog)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

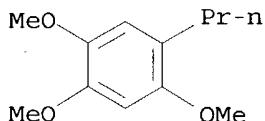


RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:740149 CAPLUS
DN 123:187711
TI Studies on crude drugs effective on visural larva migrans. XVI. Mobility
inhibition and nematocidal activity of asarone and related

09/652,376

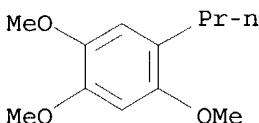
AU phenylpropanoids on second-stage larvae of *Toxocara canis*
Sugimoto, Naoki; Goto, Yoshihisa; Akao, Nobuaki; Kiuchi, Fumiuki; Kondo,
Kaoru; Tsuda, Yoshisuke
CS Sch. Med., Kanazawa Univ., Kanazawa, 920, Japan
SO Biological & Pharmaceutical Bulletin (1995), 18(4), 605-9
CODEN: BPBLEO; ISSN: 0918-6158
PB Pharmaceutical Society of Japan
DT Journal
LA English
AB The in vitro effect of asarone, the nematocidal principle of the rhizome
of *Acorus calamus*, on second-stage larvae of *Toxocara canis* is composed of
two independent actions: one is a fast acting inhibition of the larval
mobility and the other is a slow acting larvicidal action. Mobility of
the larvae was rapidly inhibited when they were incubated with asarone.
Dye exclusion assay revealed that larvae were alive at this stage, and
their mobility was restored after the first inhibition, suggesting that
this effect was temporary and reversible. However, when the mobility
decreased again during prolonged incubation, the cellular viability of
larvae disappeared, showing that they were killed by the compound. The above
two-stage effect of asarone was almost identical in two geometrical
isomers ((E)- and (Z)-asarone). Di- and tri-methoxypropenyl or
propylbenzenes carrying two methoxy groups at a vicinal position on a
benzene ring showed, more or less, a two-stage effect of this type. These
two actions were suggested to be separable by an appropriate modification
of the structure.
IT 6906-65-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); PRP (Properties); BIOL (Biological study)
(studies on crude drugs effective on visual larva migrans. XVI.
Mobility inhibition and nematocidal activity of asarone and related
phenylpropanoids on second-stage larvae of *Toxocara canis*)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



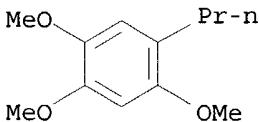
L8 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:138847 CAPLUS
DN 112:138847
TI Potential antipsychotic agents. 5. Synthesis and antidopaminergic
properties of substituted 5,6-dimethoxysalicylamides and related compounds
AU Hoegberg, Thomas; Bengtsson, Stefan; De Paulis, Tomas; Johansson, Lars;
Stroem, Peter; Hall, Haakan; Oegren, Sven Ove
CS CNS Res. Dev., Astra Res. Cent. AB, Soedertaelje, S-151 85, Swed.
SO Journal of Medicinal Chemistry (1990), 33(4), 1155-63
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 112:138847
AB A series of 3-substituted 5,6-dimethoxysalicylamides (I) have been
synthesized from the corresponding 2,5,6-trimethoxybenzoic acids.
Relaxation times T1 and carbon chemical shifts of the methoxy groups in I
showed that the 6-methoxy group adopts a nearly perpendicular orientation
and the 5-methoxy group takes on a more coplanar orientation with respect
to the ring plane in solution. The salicylamides I display a very high and
stereoselective affinity for the [3H]spiperone and [3H]raclopride binding

sites in vitro. Regioisomers of salicylamides I also exhibit pronounced, but lower than I, affinity for the [³H]spiperone binding site. The structural requirements were further assessed by studies of the related amino analogs and hydroxy analog. 3-Bromo compound II (FLB 463) was studied in various in vivo models and compared with the dopamine-D₂ antagonists sulpiride, raclopride, eticlopride, and haloperidol. The high potency of I to selectively block dopamine-D₂ receptors in vitro and in vivo combined with indications on a low potential for motor side effects makes it a very interesting new member of the class of substituted salicylamides.

IT 6906-65-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and carboxylation of)
 RN 6906-65-6 CAPLUS
 CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



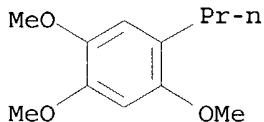
L8 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1983:517832 CAPLUS
 DN 99:117832
 TI Repellency and toxicity of 55 insect repellents to red-winged blackbirds (Agelaius phoeniceus)
 AU Schafer, E. W., Jr.; Jacobson, M.
 CS Denver Wildl. Res. Cent., USFWS, Denver, CO, 80225, USA
 SO Journal of Environmental Science and Health, Part A: Environmental Science and Engineering (1983), A18(4), 493-502
 CODEN: JESEDU; ISSN: 0360-1226
 DT Journal
 LA English
 AB A joint research program was initiated in 1979 to investigate the potential avian repellency and toxicity of 55 selected insect repellents originating from or related to naturally occurring chems. Seven of the chems. or exts. tested exhibited avian repellency and 2 of these were considered to be moderately active, with 50% avian repellency concns. of 0.237 (trans-asarone [2883-98-9]) and 0.240% (safrole [94-59-7]). None of the 55 chemical or exts. exhibited acute oral toxicity at ≤100 mg/kg to the red-winged blackbird (Agelaius phoeniceus).
 IT 6906-65-6
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
 (repellency and toxicity of, to red-winged blackbirds)
 RN 6906-65-6 CAPLUS
 CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



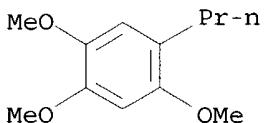
L8 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1982:100901 CAPLUS
 DN 96:100901
 TI Constituents of Acorus calamus: structure of acoramone. Carbon-13 NMR

09/652,376

AU spectra of cis- and trans-asarone
AU Patra, Amarendra; Mitra, Alok K.
CS Dep. Chem., Univ. Coll. Sci., Calcutta, 700009, India
SO Journal of Natural Products (1981), 44(6), 668-9
CODEN: JNPRDF; ISSN: 0163-3864
DT Journal
LA English
AB The phenylpropane derivs. isoeugenol Me ether, γ -asarone, cis-asarone, trans-asarone, and the new natural product acoramone (I) were isolated along with asarylaldehyde from the oil of A. calamus. The ^{13}C -NMR signal assignments of cis- and trans-asarone and their dihydroderivative are also reported.
IT 6906-65-6
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Acorus calamus)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:31614 CAPLUS
DN 70:31614
TI Isolation of 2,4,5-trimethoxyallylbenzene from Caesulia axillaries oil
AU Devgan, O. N.; Bokadia, M. M.
CS Southern Illinois Univ., Carbondale, IL, USA
SO Australian Journal of Chemistry (1968), 21(12), 3001-3
CODEN: AJCHAS; ISSN: 0004-9425
DT Journal
LA English
AB The phenolic ether obtained from the essential oil of C. axillaries has been shown to be 2,4,5-trimethoxyallyl-benzene, on the basis of chemical and spectroscopic evidence. It has tentatively been named as γ -asarone.
IT 6906-65-6P
RL: PREP (Preparation)
(from Caesulia axillaris oil)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1966:447549 CAPLUS
DN 65:47549
OREF 65:8851d-h
TI Oxa compounds. VI.
AU El'tsov, A. V.; Minkin, V. I.; Tsereteli, I. Yu.
CS Oncology Inst., Leningrad
SO Zhurnal Obshchey Khimii (1966), 2(4), 620-7

CODEN: ZOKHA4; ISSN: 0044-460X

DT Journal

LA Russian

AB cf. CA 61, 5640h; 63, 11540d. Heating 10 g. 3,4-(MeO)2C6H3OH with 7.9 g. CH2:CHCH2Br and 9 g. powdered K2CO3 in Me2CO 3 hrs. gave 56% 1-allyloxy-3,4-dimethoxybenzene, b2 114°, n20D 1.5352, which (6.35 g.) heated with 7 ml. PhNMe2 2 hrs. at 200° (bath) gave 95% crude material, which hydrogenated over Pt gave 75% 4,5-dimethoxy-2-propylphenol, m. 76°, and 2% 3,4-dimethoxy-2-propylphenol, m. 94°. The former with Me2SO4 in aqueous NaOH 40 min. gave 2,4,5-trimethoxy-1-propylbenzene, b2 114°, 1.5190. Heating 18 g. 6-hydroxy-1,4-benzodioxan with 14.5 g. CH2:CHCH2Br and 16.3 g. K2CO3 in Me2CO 3 hrs. gave 57% 6-allyloxy-1,4-benzodioxan, b2 123°, 1.5505, which heated with PhNMe2 as above 2 hrs. gave mixed allylphenols, which hydrogenated over Pt gave mixed propylphenols, which methylated with Me2SO4 in aqueous NaOH gave unseparable mixture of 6-methoxy-7-propyl-1,4-benzodioxan and the 5-Pr analog, as identified from the N.M.R. spectrum of the mixture; these were formed in approx. equal amts. To 6.3 g. AlCl3 in PhNO2 was added with ice cooling 6.6 g. 6-methoxy-1,4-benzodioxan and 3.8 g. EtCOCl in PhNO2 and on the following day gave 79% 6-methoxy-7-propionyl-1,4-benzodioxan (I), m. 81-2°, which heated with HONH2.HCl in 50% AcOH 25 min. gave 6-methoxy-7-propionamido-1,4-benzodioxan, m. 75.5-6.5°, also formed from 6-methoxy-7-amino-1,4-benzodioxan and (EtCO)2O. Reduction of I with LiAlH4 gave 6-methoxy-7-(1-hydroxypropyl)-1,4-benzodioxan, b2 163-5°. I heated with granulated Zn and HgCl2 solution in aqueous alc. HCl 4 hrs. gave 6-methoxy-7-propyl-1,4-benzodioxan,

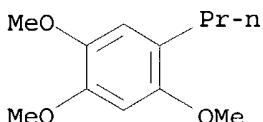
b2

131-2°, 1.5340. Elementary mol. orbital calcns. made for electron ds. in 3,4-dimethylphenol, 6-hydroxy-1,4-benzodioxan and its 5-hydroxy isomer showed differences that accounted for the differences in their chemical behavior above. The N.M.R. signals of the Me groups in 4-methylveratrole, 6-methyl-1,4-benzodioxan, its 5-Me analog, 4,5-dimethylveratrole, 6,7-dimethyl-1,4-benzodioxan, and 5,6-dimethyl-1,3-benzodioxole were reported. The last substance showed a considerable difference in spin-spin interaction of Me group protons with the various ring protons, which indicated greater degree of conductivity of conjugation effect through the 4,5-bonds in the molecule (Nair and Gopakumar, CA 60, 15701b).

IT 6906-65-6, Benzene, 1,2,4-trimethoxy-5-propyl-
(preparation of)

RN 6906-65-6 CAPLUS

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 14 OF 14 CAOLD COPYRIGHT 2004 ACS on STN

AN CA65:8851d CAOLD

TI oxa compds. - (VI)

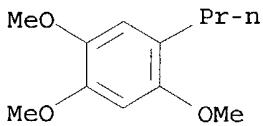
AU El'tsov, A. V.; Minkin, V. I.; Tsereteli, I. Yu.

IT 6906-65-6

RN 6906-65-6 CAOLD

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

09/652,376



=> d 14 all

L8 ANSWER 14 OF 14 CAOLD COPYRIGHT 2004 ACS on STN
AN CA65:8851d CAOLD
TI oxa compds. - (VI)
AU El'tsov, A. V.; Minkin, V. I.; Tsereteli, I. Yu.
IT 6906-64-5 6906-65-6 6906-66-7 6906-67-8 6906-68-9
6906-69-0 6906-70-3 6916-51-4 6916-52-5

=> calamus oil and hydrogenat?

CALAMUS IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s calamus oil and hydrogenat?

L9 7 CALAMUS OIL AND HYDROGENAT?

=> dup rem 19

DUPLICATE IS NOT AVAILABLE IN 'CAOLD'.

ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
PROCESSING COMPLETED FOR L9

L10 7 DUP REM L9 (0 DUPLICATES REMOVED)

=> d 1-7 bib ab

L10 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:777737 CAPLUS
DN 139:292100
TI Formation of neolignan by DDQ mediated dimerization of dihydroasarone
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi
PA Council of Scientific and Industrial Research, India
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|------------|-----------------|----------|
| PI WO 2003080551 | A1 | 20031002 | WO 2002-IN73 | 20020327 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| PRAI WO 2002-IN73 | | 20020327 | | |
| OS CASREACT | | 139:292100 | | |

09/652,376

AB The present invention relates to a novel neolignan 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-propene and a process for the preparation of high purity, high yield neolignan, α -asarone, and 2,4,5-trimethoxyphenylpropionone from β -asarone or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:777446 CAPLUS

DN 139:292099

TI DDQ-mediated one step dimerization of β -asarone or β -asarone rich Acorus calamus oil in the formation of novel neolignan

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific & Industrial Research, India

SO U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---------------------|------|----------|-----------------|----------|
| PI | US 2003187306 | A1 | 20031002 | US 2002-108269 | 20020328 |
| | US 2004049085 | A1 | 20040311 | US 2003-660556 | 20030912 |
| PRAI | US 2002-108269 | B3 | 20020328 | | |
| OS | CASREACT 139:292099 | | | | |

AB The present invention relates to a novel neolignan, 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-(2',4',5'-trimethoxy)phenyl-1-propene [NEOLASA-I (I)], and a process for the preparation of high purity, higher yield neolignan, α -asarone, 2,4,5-trimethoxy-phenylpropionone from β -asarone (II) or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

L10 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:524051 CAPLUS

DN 139:90404

TI Process for the preparation of pharmacologically active α -asarone from toxic β -asarone-rich Acorus calamus oil

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific & Industrial Research, India

SO U.S., 22 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|------|----------|-----------------|----------|
| PI | US 6590127 | B1 | 20030708 | US 2002-107844 | 20020328 |
| | WO 2003082786 | A1 | 20031009 | WO 2002-IN94 | 20020328 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,

CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2002-107844 A 20020328

AB The present invention relates to a process for the preparation of high purity and yield α -asarone, trans-2,4,5-trimethoxycinnamaldehyde, and 2,4,5-trimethoxyphenylpropanone, from β -asarone or β -asarone-rich Acorus calamus oil containing α and γ -asarone by hydrogenation, followed by treatment with a dehydrogenating agent dichlorodicyanobenzoquinone (DDQ) with or without solid support of silica gel or alumina in dry organic solvent. α -Asarone can also be obtained by treating the hydrogenated product of β -asarone or β -asarone-rich A. calamus oil with DDQ in an aqueous organic solvent to obtain an intermediate 2,4,5-trimethoxyphenylpropanone, which in turn is reduced with sodium borohydride to obtain the corresponding 2,4,5-trimethoxyphenylpropanol and followed by final treatment with a dehydrating agent.

RE.CNT 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:221245 CAPLUS

DN 136:247399

TI Process for the preparation of 1-propyl-2,4,5-trimethoxybenzene from toxic β -asarone of Acorus calamus or from crude calamus oil containing β -asarone

IN Sinha, Arun Kumar

PA Council of Scientific and Industrial Research, India

SO U.S. Pat. Appl. Publ., 16 pp., Division of U.S. Ser. No. 652,376.
CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|----------------|------|----------|-----------------|----------|
| PI | US 2002035299 | A1 | 20020321 | US 2001-957867 | 20010921 |
| | US 6528041 | B2 | 20030304 | | |
| | CN 1340494 | A | 20020320 | CN 2001-119219 | 20010327 |
| | JP 2002088004 | A2 | 20020327 | JP 2001-101894 | 20010330 |
| | US 2003113275 | A1 | 20030619 | US 2003-338327 | 20030108 |
| PRAI | US 2000-652376 | A3 | 20000831 | | |
| | US 2001-957867 | A3 | 20010921 | | |

OS CASREACT 136:247399

AB The invention relates to a process for the preparation of 1-Propyl-2,4,5-trimethoxybenzene useful as a aroma mol. and as a starting material and intermediate for preparation of various drugs. The process comprises providing crude calamus oil or β -asarone in a solvent; hydrogenating the solution in the presence of a catalyst; filtering the catalyst and removing the solvent under reduced pressure; subjecting the reduced calamus oil to column of silica gel chromatog. using an eluent to obtain the desired product in liquid form with 85-97% purity.

L10 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1987:72677 CAPLUS

DN 106:72677

TI Isolation and synthesis of (Z,Z)-4,7-decadienal, the character impact compound in the oil of Acorus calamus L

AU Van Lier, F. P.; Van der Linde, L. M.; Van der Weerdt, A. J. A.

CS Org. Res. Dep., Naarden Int., Bussum, 1400 CA, Neth.

SO Prog. Essent. Oil Res., Proc. Int. Symp. Essent. Oils, 16th (1986), Meeting Date 1985, 215-25. Editor(s): Brunke, Ernst-Joachim. Publisher: de Gruyter, Berlin, Fed. Rep. Ger.

CODEN: 55BIAR
 DT Conference
 LA English
 AB A number of aldehydes, many not previously found, were isolated from A. calamus oil. The syntheses of (Z,Z)-4,7-decadienol (I) [104188-11-6], (Z)-4- [68820-32-6] and (Z)-5-undecenal [68464-53-9], (Z,Z)-4,7-undecadienol [104188-12-7], and (E)-2-butyl-2-octenal [64935-38-2] were carried out for proof of structure and to correlated odors of the oils with the compds. Thus, I was prepared by ozonolysis of (Z,Z)-1,5-cyclooctadiene followed by oxidation with FeCl₃ of the methoxy hydroperoxide to give (Z)-C₁CH₂CH₂CH:CHCH₃CH₂CH(OMe), iodine exchange, treatment with Ph₃P and Wittig reaction of (Z)-Ph₃P+CH₂CH₂CH:CHCH₂CH(OMe)₂ with the appropriate aldehydes. A number of other aldehydes were prepared with this Wittig compound. The odor of I most closely resembled that of A. calamus oil.

L10 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1955:86792 CAPLUS
 DN 49:86792
 OREF 49:16355h-i,16356a-c
 TI Advancements in the chemistry of sesquiterpenes
 AU Sorm, Frantisek
 SO Magyar Tudomanyos Akad. Kemial Tudomanyok Osztalyanak Kozlemenyei (1953), 3, 351-66
 DT Journal
 LA Unavailable
 AB cf. C.A. 47, 9944c. Sesquiterpene hydrocarbons were isolated and identified by distillation combined with chromatographic adsorption on alkaline Al₂O₃ and infrared spectrophotometry. It is possible to sep. sesquiterpenes differing in number of double bonds or in C skeletons. The infrared spectra of caryophyllene from clove oil, oil of wormwood, and oil of bergamot were compared with the spectra of γ -cadinene and δ -cadinene from oil of citronella ϵ -cadinene from ylang-ylang oil, cadinene regenerated from 1-cadinene-HCl, tetrahydro- γ -cadinene, tetrahydro- δ -cadinene, and cadinane from regenerated cadinene. The explanation of structures of unknown compds. was aided by hydrogenation and elimination of functional groups of the sesquiterpenes in order to compare the skeleton with known saturated hydrocarbons. By this method the structures of 2 diterpene hydrocarbons, C₂₀H₃₀ and C₂₀H₃₂, isolated from oil of wormwood were clarified. The infrared spectra of the partially hydrogenated aromatic diterpene, C₂₀H₃₀, were shown to be similar to that of 2,6-dimethyl-10-(p-tolyl)undecane. The structures of monocyclic sesquiterpenes of the bisabolane, humulene, and elemol (I) type were discussed. The skeleton of I appears to be 1-methyl-1-ethyl-2,4-diisopropylcyclohexane. Dicyclic sesquiterpenes such as cadinene, calacorene, caryophyllene, caratol, chamazulene, and the isomeric acorone and isoacorone (from calamus oil) were discussed and structures suggested for them.

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 AU Sorm, Frantisek
 CS Stockholm
 SO XIIIth Intern. Congr. Pure Appl. Chem. (1953), (Collection Czechoslov. Chem. Commun. Suppl. 2), 19, 68-80
 DT Journal
 LA German
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identified by distillation combined with chromatographic adsorption on alkaline Al₂O₃ and infrared spectrophotometry. It is possible to sep. sesquiterpenes differing in number of double bonds or in C skeletons. The infrared spectra of caryophyllene from clove oil, oil of wormwood, and oil of bergamot were compared with the spectra of γ -cadinene and δ -cadinene from oil of citronella ϵ -cadinene from ylang-ylang oil, cadinene regenerated from 1-cadinene-HCl, tetrahydro- γ -cadinene, tetrahydro- δ -cadinene, and cadinane from regenerated cadinene. The explanation of structures of unknown compds. was aided by hydrogenation and elimination of functional groups of the sesquiterpenes in order to compare the skeleton with known saturated hydrocarbons. By this method the structures of 2 diterpene hydrocarbons, C₂₀H₃₀ and C₂₀H₃₂, isolated from oil of wormwood were clarified. The infrared spectra of the partially hydrogenated aromatic diterpene, C₂₀H₃₀, were shown to be similar to that of 2,6-dimethyl-10-(p-tolyl)undecane. The structures of monocyclic sesquiterpenes of the bisabolane, humulene, and elemol (I) type were discussed. The skeleton of I appears to be 1-methyl-1-ethyl-2,4-diisopropylcyclohexane. Dicyclic sesquiterpenes such as cadinene, calacorene, caryophyllene, caratol, chamazulene, and the isomeric acorone and isoacorone (from calamus oil) were discussed and structures suggested for them.

=> log y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 110.54 | 423.36 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -14.70 | -14.70 |

STN INTERNATIONAL LOGOFF AT 18:02:22 ON 19 AUG 2004